SECTION I. INTRODUCTION

I.A. Program Background and Description

During the past 5 years, significant advances have been made at Brigham Young University (BYU) in comprehensive two-dimensional computer codes for mechanistic modeling of entrained-bed gasification and pulverized coal combustion. During the same time period, significant advances have been made at Advanced Fuel Research, Inc. (AFR) in the mechanisms and kinetics of coal pyrolysis and secondary reactions of pyrolysis products. The proposed program presents a unique opportunity to merge the technology developed by each organization to provide detailed predictive capability for advanced coal conversion processes. This predictive capability will incorporate advanced coal characterization techniques in conjunction with comprehensive computer models to provide accurate process simulations.

The program will streamline submodels existing or under development for coal pyrolysis chemistry, volatile secondary reactions, tar formation, soot formation, char reactivity, and SO_x-NO_x pollutant formation. Submodels for coal viscosity, agglomeration, tar/char secondary reactions, sulfur capture, and ash physics and chemistry would be developed or adapted. The submodels would first be incorporated into the BYU entrained-bed gasification code and subsequently, into a fixed-bed gasification code (to be selected and adapted). These codes would be validated by comparison with small scale laboratory and PDU-scale experiments. The validated code could then be employed to simulate and to develop advanced coal conversion reactors of interest to METC.

I.B. Objectives

The objectives of this proposed study are to establish the mechanisms and rates of basic steps in coal conversion processes, to integrate and incorporate this information into comprehensive computer models for coal conversion processes, to evaluate these models and to apply them to gasification, mild gasification and combustion in heat engines.

I.C. Approach

This program will be a closely integrated, cooperative effort between AFR and BYU. The program will consist of four tasks: 1) Preparation of Research Plans, 2)

Submodel Development and Evaluation, 3) Comprehensive Model Development and Evaluation, and 4) Applications and Implementation.

I.D. Critical Technical Issues

To achieve the goals of the program, the computer models must provide accurate and reliable descriptions of coal conversion processes. This will require the reduction of very complicated and interrelated physical and chemical phenomena to mathematical descriptions and subsequently to operational computer codes. To accomplish this objective a number of technical issues must be addressed as noted below.

I	Separation of Rates for Chemical Reaction, Heat Transfer, and Mass Transfer
I	Particle Temperature Measurements Using FT-IR E/T Spectroscopy
I	Functional Group Description of Coal, Char, and Tar
I	Tar Formation Mechanisms
I	Char Formation Mechanisms
I	Intraparticle Transport
I	Pyrolysis of Volatiles and Soot Formation
I	Secondary Reaction of Tar
●	Particle Ignition
I	Ash Chemistry and Physics
I	Particle Optical Properties
I	Code Efficiency and Compatibility for Submodels
I	Coupling of Submodels with Comprehensive Codes
I	Comprehensive Code Efficiency
I	Turbulence
I	SO_x and NO_x
●	Generalized Fuels Model
I	Fixed-Bed Model

(●) to be addressed; (I) initiated; (C) completed.

These technical issues are addressed in the three Tasks as described in Section II-IV.

I.E. Second Quarter Progress

SUBTASK 2.a. Coal to Char Chemistry Submodel

The literature search on transport properties during pyrolysis was completed. Work was initiated on computing the optical properties of particles during the coal to char transformations. A paper was prepared for Combustion and Flame. Characterizations of the coals which will be used for this program were performed using FT-IR, TGA, and pyrolysis tests.

SUBTASK 2.b. Fundamental High-Pressure Reaction Rate Data

The research team was organized and consists of two senior investigators, a doctoral student and an undergraduate research assistant. A second graduate student is being sought. Development of the detailed experimental program was initiated, and design of a small-scale high pressure reactor was also begun.

SUBTASK 2.c. Secondary Reactions of Pyrolysis Products and Char Burnout Submodels

Studies of ignition were begun in the transparent wall reactor (TWR). Attention was focused on what controls ignition - heterogeneous or homogeneous oxidations, The initial evidence points on the latter. A paper was prepared on the initial observations for the International Coal Combustion Symposium.

SUBTASK 2.d. Ash Physics and Chemistry Submodel

A literature review was started on the effect of mineral matter in gasification. An ash collection was designed and constructed for the TWR.

SUBTASK 2.e. Large Particle and Chemistry Submodel

Initial work was performed on defining the regions of temperature and heating rate dominated by kinetics, heat transfer and mass transfer limitations.

SUBTASK 2.g. SO_x-NO_x Submodel Development

A graduate research assistant for this subtask was recruited. The graduate assistant attended the 1987 NO_x Control Conference. Independent work on development of a SO_x-sorbent capture submodel was reviewed. Work also continued on

an independently sponsored project to evaluate the NO_x submodel.

SUBTASK 2.h. NO_x/SO_x Submodel Evaluation

A graduate student interested in the cold-flow portion of the study was identified and hired. He has begun to familiarize himself with the LDV instrument. David Pershing (University of Utah) has been contacted, and has agreed to help locate information on the design characteristics of a commercial electric power plant that will be using sorbent injection downstream of the burner injection point.

SUBTASK 3.a. Integration of Advanced Submodels into Entrained-Flow Code, with Evaluation and Documentation

An effort to recruit a graduate student was initiated. A literature review and code calculations were initiated to better understand the FG/DVC models and how they might best be incorporated into PCGC-2. A contract review meeting was conducted at BYU.

SUBTASK 3.b. Comprehensive Fixed-Bed Modeling Review, Development Evaluation and Implementation

A potential graduate student has been identified to work on this subtask. A partial list of existing codes and criteria for evaluating the codes has been identified.

SUBTASK 4.a. Application of Generalized Pulverized Coal Comprehensive Code

PCGC-2 was installed on AFR's Apollo DN 580. The code without the NO_x model is now operational.

SUBTASK 4.b. Application of Fixed-Bed Code

No work was scheduled.